A constraint on a varying proton–electron mass ratio 1.5 billion years after the Big Bang: Supplemental Material

J. Bagdonaite, W. Ubachs
Department of Physics and Astronomy, and LaserLaB, VU University, De Boelelaan 1081, 1081 HV Amsterdam, The Netherlands

M. T. Murphy, J. B. Whitmore
Centre for Astrophysics and Supercomputing, Swinburne University of Technology, Melbourne, Victoria 3122, Australia
(Dated: January 22, 2015)

FITTED TRANSITIONS

In Table I, the 89 fitted H_2 transitions are listed, grouped by the ground J level. Of these transitions, 17 are from the Werner band. The fitted regions are displayed in Fig. 1 to 4.

TABLE I. 89 fitted H_2 transitions in 60 regions of the J1443+2724 spectrum.

J level	Number of tr.	Transition names
0	7	W3R(0), L14R(0), L10R(0), L8R(0), L7R(0), L1R(0), L0R(0)
1	20	L16P(1), L15P(1), L15R(1), W3R(1), L12R(1), L12P(1), W2Q(1), L10R(1), L10P(1), L9R(1), L9P(1), L8P(1), L4R(1), L4P(1), L3R(1), L3P(1), L2R(1), L2P(1), L1R(1), L1P(1)
2	27	L16R(2), L15R(2), L13R(2), L12P(2), W2R(2), W2Q(2), W2P(2), L11R(2), L11P(2), L10P(2), W1R(2), W1Q(2), L9R(2), L9P(2), L8R(2), W0Q(2), L7R(2), L6P(2), L5P(2), L4R(2), L4P(2), L3P(2), L2R(2), L2P(2), L1R(2), L1P(2), L0P(2)
3	26	L15R(3), W3P(3), L13R(3), L13P(3), L12R(3), W2R(3), L12P(3), W2Q(3), W2P(3), L11P(3), L10R(3), L10P(3), W1R(3), L9R(3), W0R(3), W0Q(3), L6R(3), L5P(3), L4R(3), L4P(3), L3R(3), L3P(3), L2R(3), L1R(3), L0R(3)
4	9	L17P(4), L16P(4), L15R(4), L13P(4), L12R(4), L11P(4), W1Q(4), L9P(4), W0Q(4)

CONTINUUM ERROR

One possible source of uncertainty in $\Delta\mu/\mu$ can in principle be caused by incorrect treatment of the continuum; we address it here. One can assume that, for 60 fitted sections (containing the 89 H_2 lines), the continuum error is random, with the error in the slope of the continuum over any individual H_2 section (of width ~100 km/s) being Gaussian-distributed with a sigma of approximately 0.05 [norm. flux units] / 100 km/s = 5×10^{-4} per km/s. Individual H_2 transitions are ~40 km/s wide in this absorber, so this corresponds to an incorrect continuum slope of $\sim2\times10^{-3}$ across the transition. To a reasonable approximation, this should impart a spurious shift to the fitted centroid of 0.002 times the width, i.e. 40 km/s again, or a shift of ~ 80 m/s for an individual line. Some of the 89 lines are blended together and therefore share the same spurious shift. Thus, effectively a sample of ~70 transitions reduces the per-line error of 80 m/s down to a total error budget of $80/\sqrt{70} \approx 10$ m/s, which is well below our systematic or random error budgets.

The global quasar continuum assumed initially is just a nominal starting guess which is refined by introducing local continua to each fitting region. These local continua are either constants or straight lines so that degeneracies with broad Ly-α lines would be avoided. Therefore, errors in the global continuum level in each fitting section are marginalized over by fitting a local continuum with a slope and also fitting the broader HI Ly-α lines.

VARYING THE MINIMUM LINEWIDTH PARAMETER

The minimum linewidth paramater $b_{\rm min}$ in VPFIT is user-defined. Throughout the paper, we use a $b_{\rm min}$ = 0.2 km/s. In the case of J1443+2724, one of the H_2 velocity components reaches this limit. This is likely unphysical because $b_{\rm H2} = 0.2$ km/s corresponds to $T \sim 5$ K, while the temperature of the Cosmic Microwave Background radiation at $z = 4.224$ corresponds to $T = 14$ K or $b_{\rm H2} = 0.3$ km/s. Furthermore, the kinetic temperature in cold molecular clouds is typically around ~ 100 K or

$b_{\rm H2} = 0.9$ km/s. In Fig. 5, we show how imposing these values as $b_{\rm min}$ affects $\Delta\mu/\mu$. Overall, the resulting $\Delta\mu/\mu$ values are in agreement with the fiducial $\Delta\mu/\mu$ limit from the 3VC model with $b_{\rm min} = 0.2$ km/s. However, the goodness of fit parameter χ^2_ν increases with increasing $b_{\rm min}$ values. For example, a χ^2_ν of 1.161 results from the 3VC model with $b_{\rm min} = 0.2$ km/s, and $\chi^2_\nu = 1.189$ from the same model with $b_{\rm min} = 0.9$ km/s. This indicates that the former model is statistically preferred over the latter.

SUPERCALIBRATION

Long-range wavelength distortions in UVES can be quantified by means of a so-called supercalibration method which is based on observations of objects with well understood spectra [19, 32]. In particular, these objects can be asteroids or solar twins which both exhibit solar-like spectra. Their observations include the usual ThAr calibration routine, used also for the quasar, and the resulting spectra are compared to a highly accurate solar spectrum obtained by an independent instrument, namely Fourier Transform Spectrometer (FTS). The comparison provides means to verify correctness of the ThAr calibration and to make adjustments if it is found to be flawed.

In Table II, observational details are provided regarding the J1443+2724 observing runs both in 2004 and 2013. The service mode J1443+2724 observations were conducted during 2-3 and 17-19 of March, 2004. Note that most of the total SNR of the J1443+2724 spectrum originates from this dataset (see Table III). Even though dedicated asteroid or solar twin observations were not carried out along with the quasar observations, incidentally, on the ESO archive [33] we could find several sun-like stars observed during that time period under a different program; their observational details are collected in Table IV. It has to be noted that even though the same arm of the spectrograph was used, the settings of the quasar observations and those of the sun-like stars were not identical. By applying the supercalibration method described above, we found corrections amounting to 44.9±46.8 m/s/1000Å (see Fig. 6). Here we assume that the distortions remain semistable over time periods as long as several weeks, and that the slopes obtained from the solar twins hold also for the main target. The resulting $\Delta\mu/\mu$ correction is quoted in the manuscript.

Asteroids Juno and Flora, and the solar twin HD126525 were observed along with J1443+2724 in March 2013. The instrumental settings of the quasar observations were maintained during the observations of calibration sources: a 544 or 520 nm central wavelength, 2x2 CCD binning, 0.8″ slit. For this sample of solar-like spectra, a significant deviation from perfect calibration was found with an average slope value of the correction amounting to 297.6 ± 122.7 m/s/1000Å. In a study of H_2 toward B0642−5038, a miscalibration of similar size yielded a $\Delta\mu/\mu$ correction of -10×10^{-6} [24]. Fitting the uncorrected 2013 subspectrum results in $\Delta\mu/\mu = (4.0 \pm 12.4) \times 10^{-6}$ for the 3VC model. If a correction is applied a $\Delta\mu/\mu$ of $(-9.3 \pm 12.4) \times 10^{-6}$ is obtained. Because of a low SNR, it is difficult to reliably estimate the uncertainty of this shift. Hence, we do not correct the present 2013 subspectrum of J1443+2724.

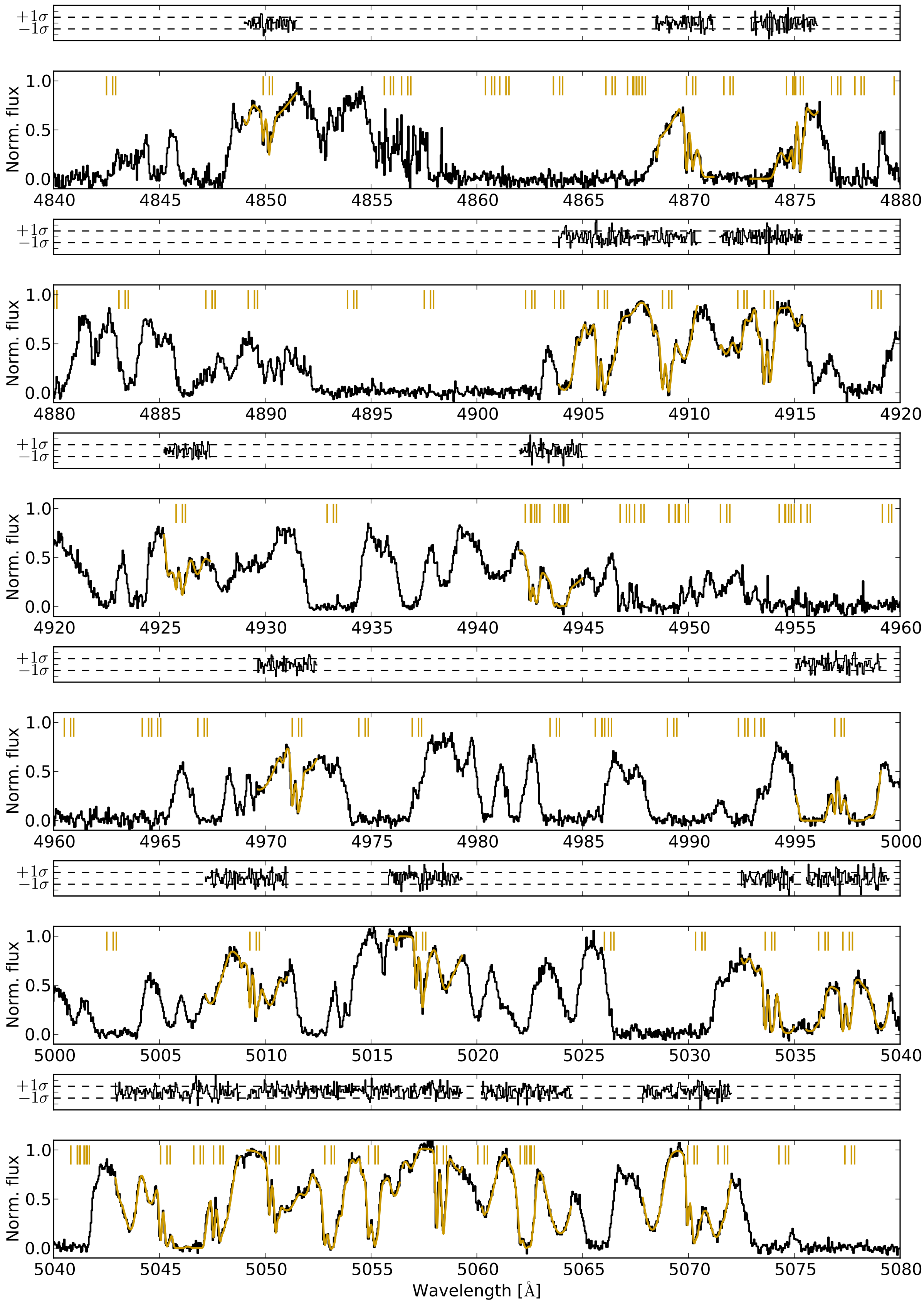

FIG. 1. Spectrum of the J1443+2724 quasar with the fitted H_2 absorption lines at redshift $z = 4.224$ (part 1 of 4). The vertical tick marks indicate positions of the velocity components for the $J = (0-4)$ transitions in the 3 VC model.

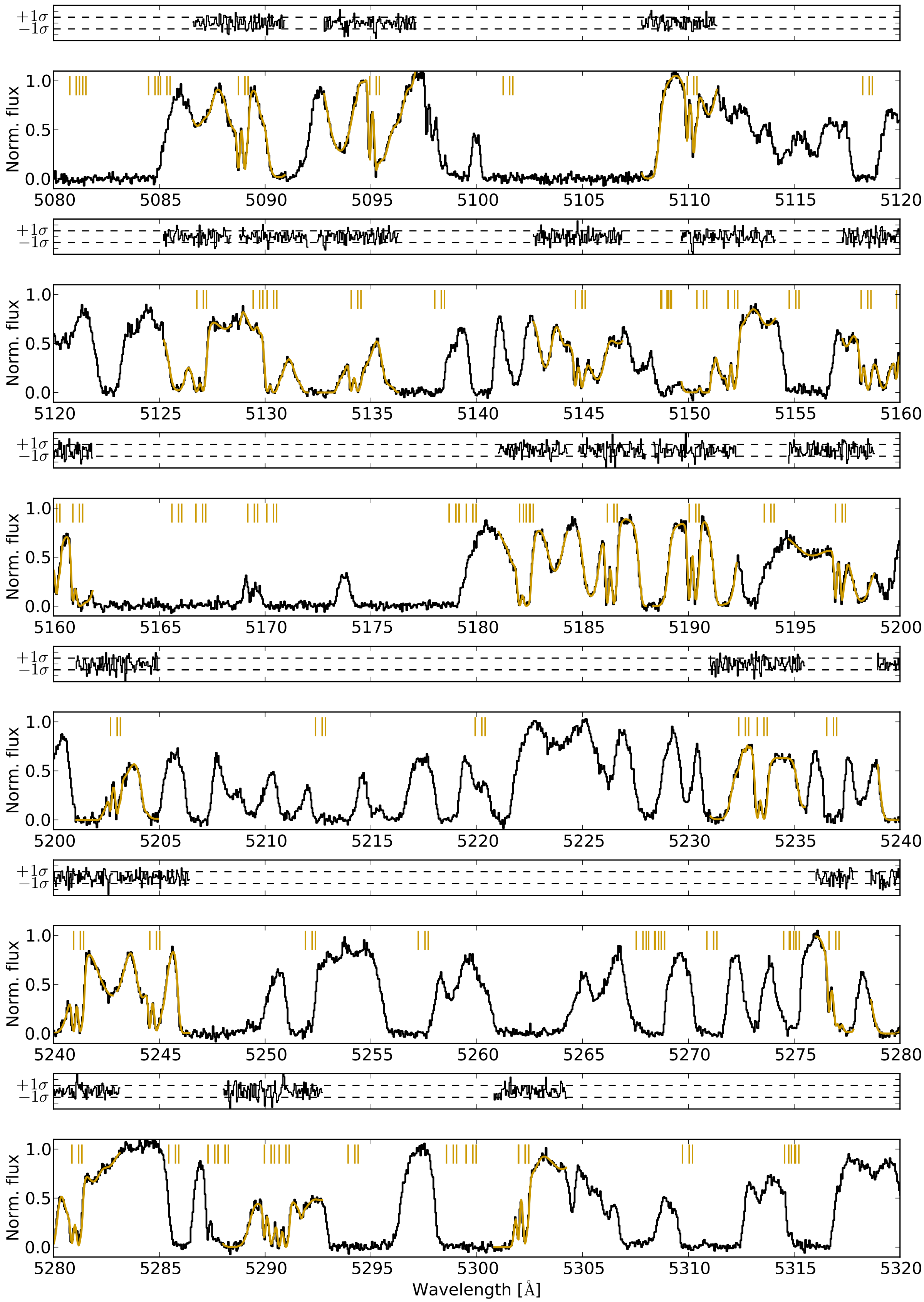

FIG. 2. Spectrum of the J1443+2724 quasar with the fitted H_2 absorption lines at redshift $z = 4.224$ (part 2 of 4).

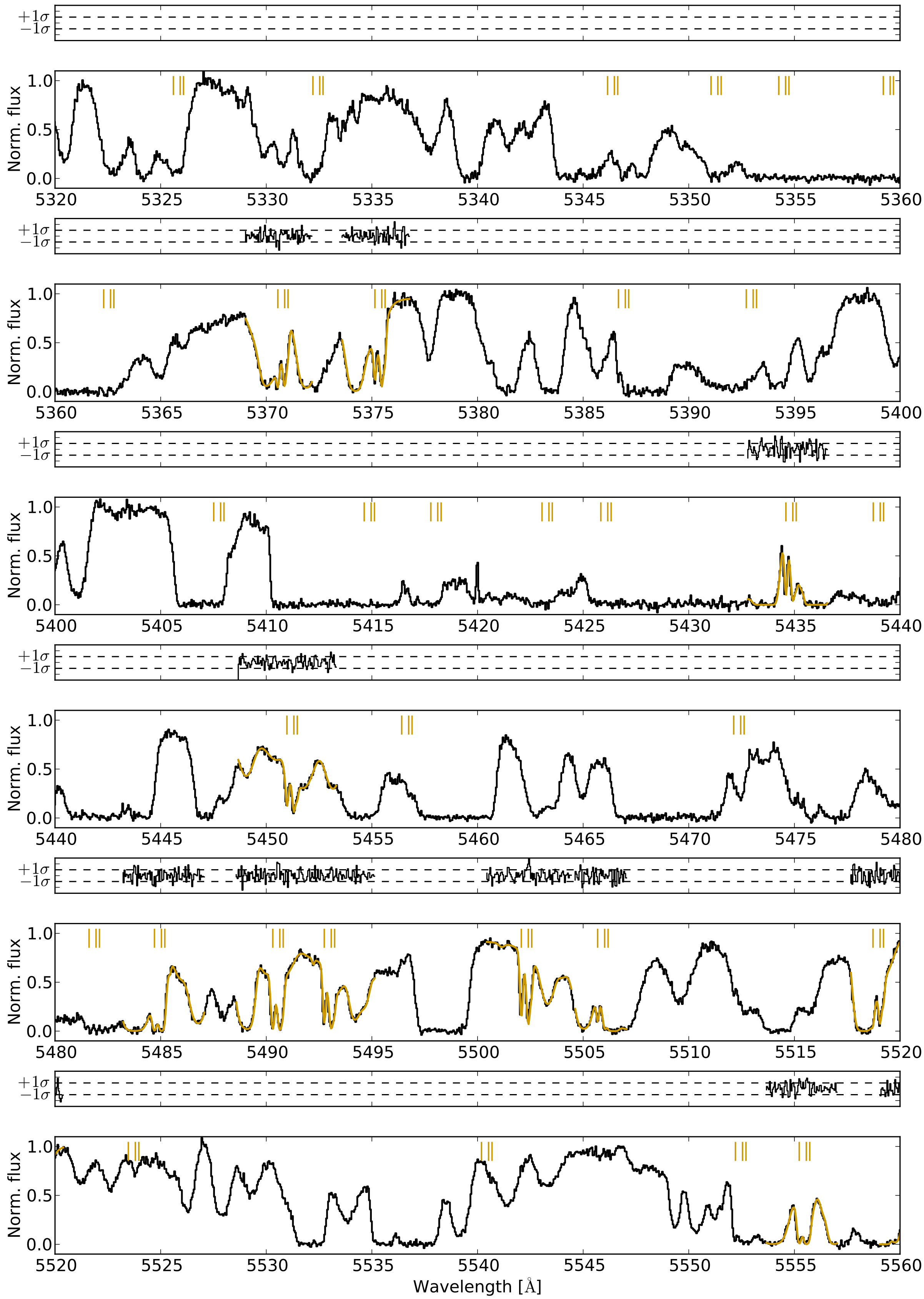

FIG. 3. Spectrum of the J1443+2724 quasar with the fitted H_2 absorption lines at redshift $z = 4.224$ (part 3 of 4).

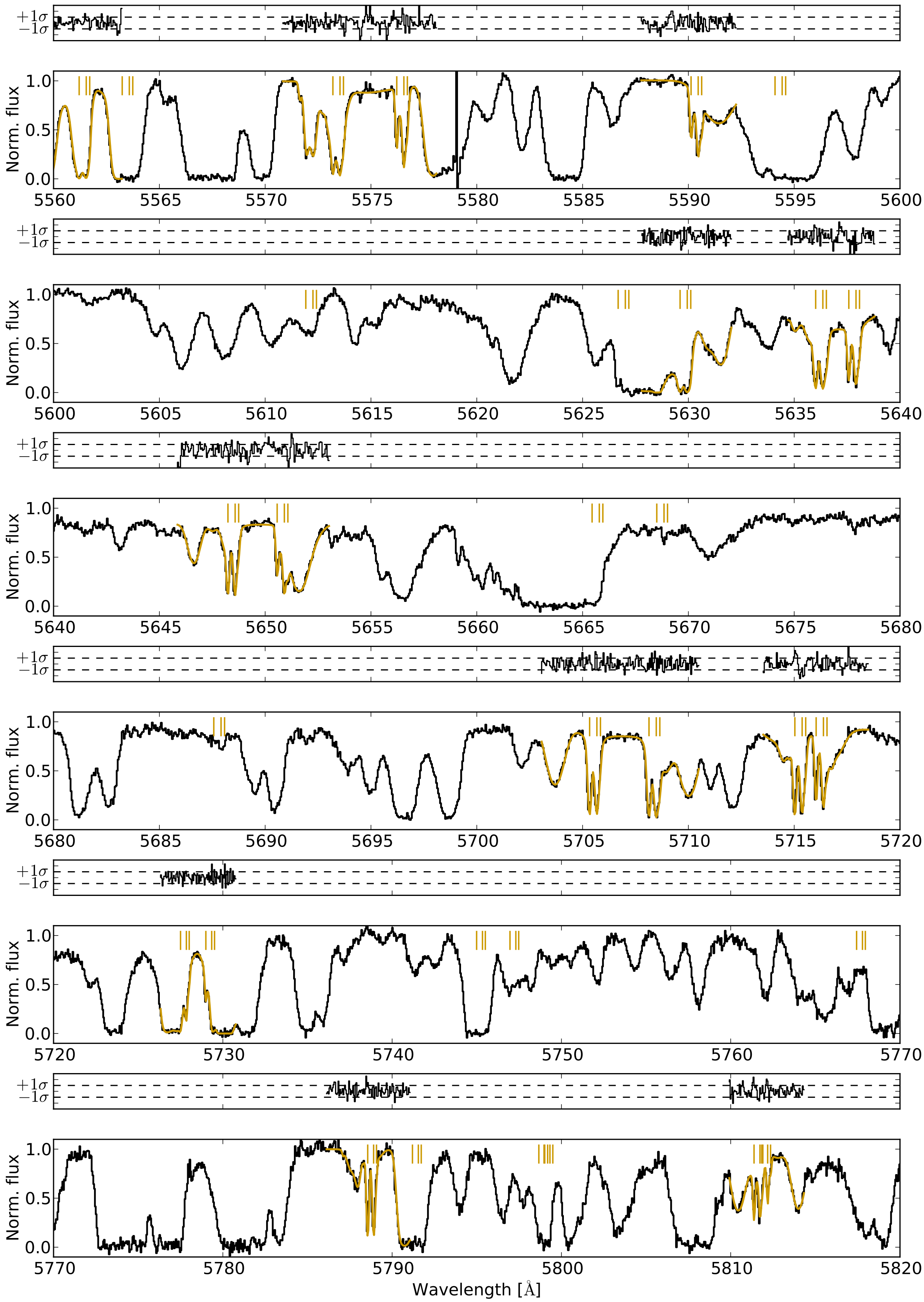

FIG. 4. Spectrum of the J1443+2724 quasar with the fitted H_2 absorption lines at redshift $z = 4.224$ (part 4 of 4).

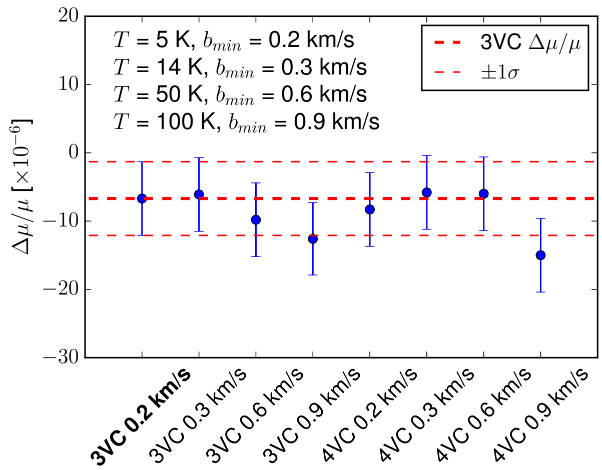

FIG. 5. Results of fitting the J1443+2724 spectrum with different minimum width parameter $b_{\rm min}$. For the H_2 molecule, the Cosmic Microwave Background radiation at $z = 4.224$ corresponds to $T = 14$ K. The kinetic temperature in cold molecular clouds typically amounts to $50 - 100$ K.

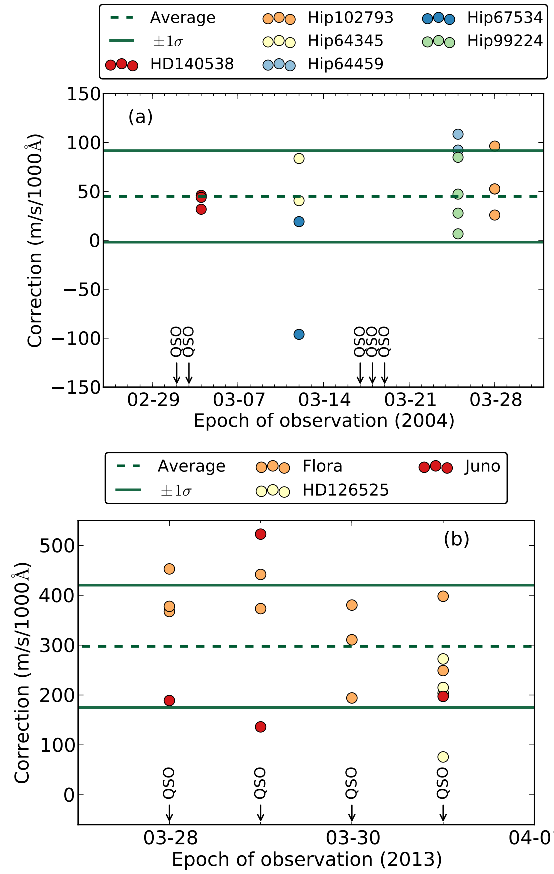

FIG. 6. (a) Supercalibration results from 2004. The average correction value amounts to 44.9±46.8 m/s/1000Å. (b) Supercalibration results from 2013. The average correction value amounts to 297.6±122.7 m/s/1000Å.

TABLE II. ESO archival data of the J1443+2724 observations with VLT/UVES (program IDs: 072.A-0346(B) and 090.A-0304(A)). The archival exposure name contains the date and time of the observations.

Archival exposure name	Central wavelength [nm]	CCD binning	Slitwidth [″]	Integ. time [s]
UVES.2004-03-02T07:52:43.078.fits	580	2x2	1.0	5225.00
UVES.2004-03-03T08:12:39.143.fits	580	2x2	1.0	5016.00
UVES.2004-03-17T08:14:13.810.fits	580	2x2	1.0	5091.00
UVES.2004-03-18T06:53:02.273.fits	580	2x2	1.0	5225.00
UVES.2004-03-19T06:35:36.823.fits	580	2x2	1.0	5800.00
UVES.2013-03-28T05:15:58.805.fits	544	2x2	0.8	4800.00
UVES.2013-03-28T06:39:39.743.fits	544	2x2	0.8	4800.00
UVES.2013-03-28T08:02:50.876.fits	544	2x2	0.8	4800.00
UVES.2013-03-29T05:22:20.681.fits	544	2x2	0.8	4800.00
UVES.2013-03-29T06:45:12.579.fits	544	2x2	0.8	4800.00
UVES.2013-03-29T08:10:27.130.fits	544	2x2	0.8	4800.00
UVES.2013-03-30T05:03:29.905.fits	520	2x2	0.8	4800.00
UVES.2013-03-30T06:28:32.340.fits	520	2x2	0.8	4800.00
UVES.2013-03-30T07:51:11.513.fits	520	2x2	0.8	6000.00
UVES.2013-03-31T05:03:05.640.fits	544	2x2	0.8	4800.00
UVES.2013-03-31T06:25:58.450.fits	544	2x2	0.8	4800.00
UVES.2013-03-31T07:49:11.563.fits	544	2x2	0.8	6300.00

TABLE III. Representative signal-to-noise (SNR) values measured in the continuum of the J1443+2724 spectrum. The red-shifted H_2 transitions are found in the range between 484 and 581 nm. The total spectrum is a combination of two datasets obtained independently in 2004 and 2013. The SNR at shorter wavelengths is entirely dominated by the data from 2004 as the observations in 2013 were affected by the full Moon.

λ [nm]	SNR_{tot}	SNR_{2004}
501.5	25	23
528.5	30	26
560.0	48	39

TABLE IV. ESO archival data of several sun-like stars observed in 2004 (program IDs: 072.D-0739(A) and 072.B-0179(A)), at a similar time when also part of the J1443+2724 data were taken. The archival exposure name contains the date and time of the observations.

Target	Archival exposure name	Central wavelength [nm]	CCD binning	Slitwidth [″]
HD140538	UVES.2004-03-04T08:11:03.429.fits	860	2x2	1.0
HD140538	UVES.2004-03-04T08:11:06.685.fits	390	2x2	1.0
Hip64345	UVES.2004-03-12T07:14:53.472.fits	564	1x1	0.3
Hip67534	UVES.2004-03-12T08:09:56.593.fits	564	1x1	0.3
Hip64459	UVES.2004-03-25T07:43:09.439.fits	564	1x1	0.3
Hip64459	UVES.2004-03-25T07:46:30.774.fits	564	1x1	0.3
Hip99224	UVES.2004-03-25T09:12:28.662.fits	564	1x1	0.3
Hip99224	UVES.2004-03-25T09:22:46.173.fits	564	1x1	0.3
Hip102793	UVES.2004-03-28T09:01:15.687.fits	564	1x1	0.3
Hip102793	UVES.2004-03-28T09:17:43.306.fits	564	1x1	0.3